Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.58 days

Global applicability domain: Outside

Local applicability domain index: 3.49e-01

Confidence level: 8.17e-01

Nearest Neighbors from the Training Set

Image not found
Pentane
Measured: 40.7
Predicted: 6.52

Image not found
2-Methylhexane
Measured: 12.5
Predicted: 5.54

Image not found
n-Hexane
Measured: 157
Predicted: 7.45

Image not found
2-Methylheptane
Measured: 12.5
Predicted: 3.99

Image not found
2-Methyloctane
Measured: 40.7
Predicted: 4.23